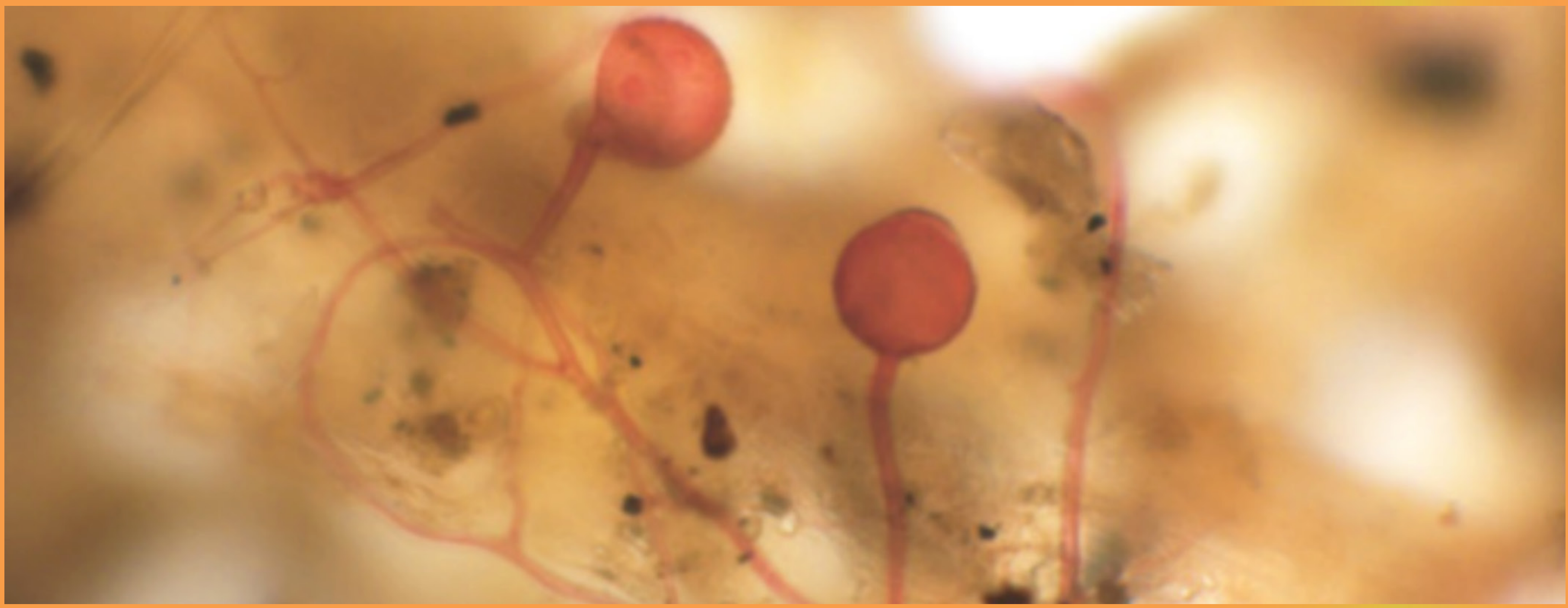
Science and Technology UPDATE

March–May 2013



Science on a Mission

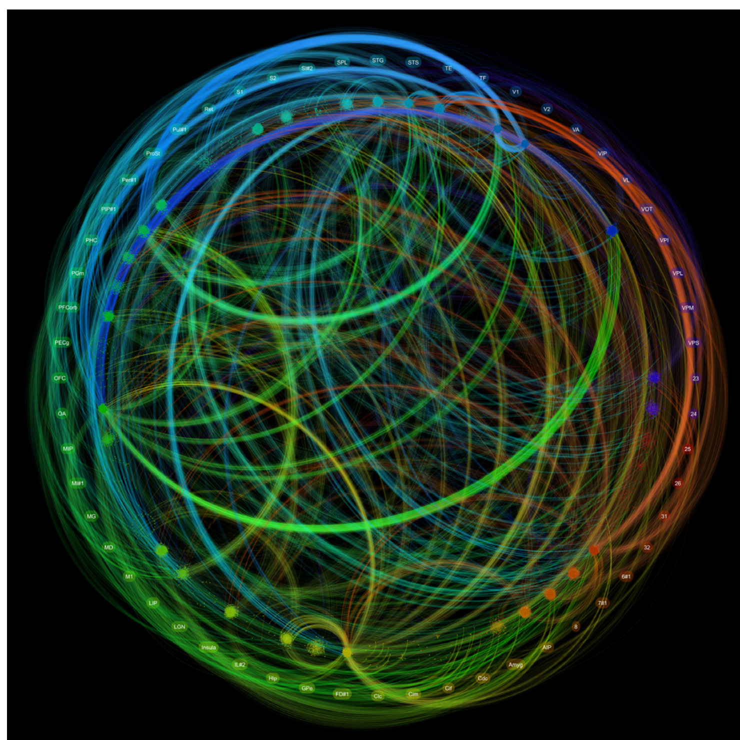
LLNL-MI-638132

LAWRENCE FELLOW WINS EUROPEAN PHYSICAL SOCIETY PH.D. AWARD

Lawrence fellow Frederico Fiuza is one of three recipients of this year's Ph.D. Research Award from the Plasma Physics Division of the European Physical Society (EPS). Frederico will be presented with his award at the 40th EPS Conference on Plasma Physics, **to be held** in Helsinki, Finland, July 1–5. Frederico received the award for the work on his doctoral thesis, *Multiscale PIC Simulations of High-Energy-Density Scenarios: from Laboratory to Astrophysics*. His thesis research spanned several topics, from multiscale particle-in-cell simulations of the fast ignition of fusion targets to the study of collisionless shocks and particle acceleration from laser–plasma interactions under laboratory conditions. Frederico said, "It is an honor to be selected for this award from the European Physical Society and an extra motivation to do quality research." The **EPS Ph.D. Research Award** was created in 2005 and is awarded annually to Ph.D. work of exceptional quality in plasma physics by a graduate student working in an EPS member state. The award is a key element of EPS Plasma Physics Division activities to recognize exceptional work by young scientists.

"ARTIFICIAL BRAIN" REACHES MILESTONE ON SEQUOIA

Being developed under DARPA's Systems of Neuromorphic Adaptive Plastic Scalable Electronics (**SyNAPSE**) initiative, the IBM brain-simulating TrueNorth system **reached** a key milestone running on the Laboratory's Blue Gene/Q Sequoia—simulating 530 billion neurons and 100 trillion synapses. This makes the system the most powerful brain simulation ever. Thanks to Sequoia's power and speed, the simulation ran only 1,542 times slower than real time, which is quite fast in the computing world. This achievement **was presented** at the Supercomputing 2012 conference. The image (courtesy of IBM) shows a network of neurosynaptic cores derived from the world's largest "wiring diagram" of a monkey's brain, which maps long-distance connections in the brain.



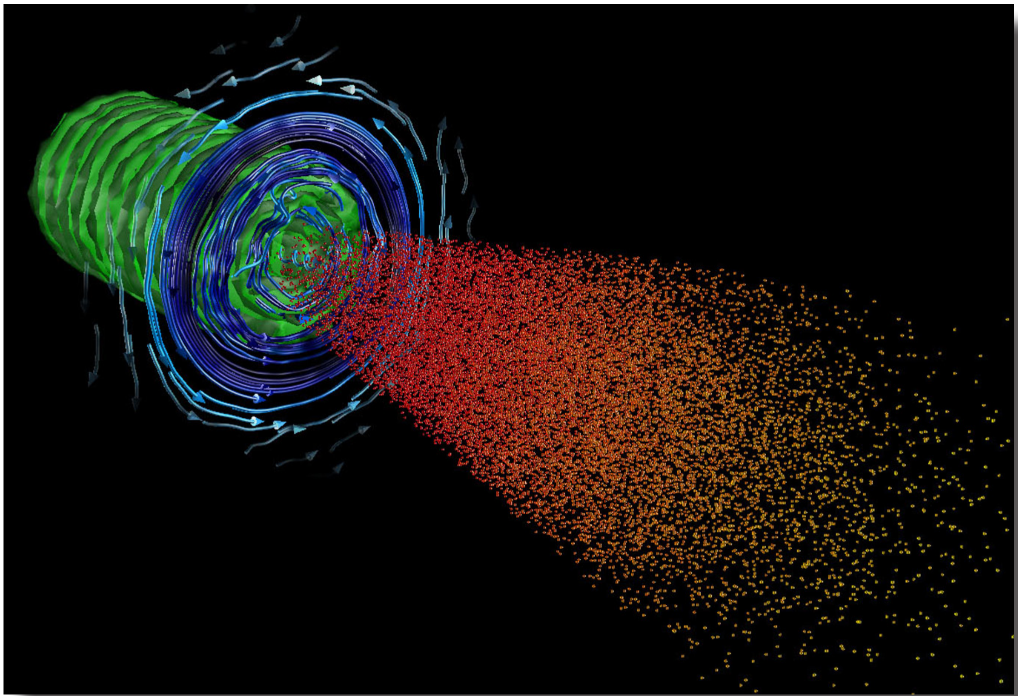
About the Cover

Arbuscular micorrhizal fungi live in symbiosis with many plants—a relationship that has been found to play a key role in carbon and nitrogen cycling. (See "Plant–fungus symbiosis shown to play role in carbon and nitrogen cycling", on page 17.)

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-7NA27344.

SEQUOIA, FIRING ON ALL CORES, SETS SUPERCOMPUTING RECORD

Lawrence Fellow Frederico Fiuza and colleagues in the Lab's Fusion Energy Sciences Program have performed record simulations using all 1,572,864 cores of the Sequoia. The simulations are the largest (by number of cores used) particle-in-cell (PIC) code simulations ever performed. PIC simulations are used extensively in plasma physics to model the motion of the charged particles—and the electromagnetic interactions between them—that make up ionized matter. In this case, the simulations were carried out to model the interaction of realistic-scale lasers with dense plasmas in three dimensions to explore a large parameter space and optimize the design for the fast-ignition approach to inertial confinement fusion. Each simulation tracks the dynamics of more than 100 billion particles for more than 100,000 computational time steps. This is approximately an order of magnitude larger than the previous largest simulations of fast ignition. These simulations made use of OSIRIS, a PIC code that was developed over more than 10 years in a collaboration between UCLA and Portugal's Instituto Superior Técnico. Frederico demonstrated excellent scaling in parallel performance of OSIRIS to the full ~1.6 million cores of Sequoia: in increasing the number of cores for a problem of fixed size (strong scaling), OSIRIS obtained 75 percent efficiency on the full machine; while increasing the total problem size (weak scaling), a 97 percent efficiency was achieved. This implies that a simulation that takes an entire year to perform on a medium-sized cluster of 4,000 cores can now be performed in a single day on Sequoia. This work was supported by funding from the DOE Office of Science's Office of Fusion Energy Science. The figure shows an OSIRIS simulation on Sequoia of the interaction of a fast-ignition-scale laser with a dense deuterium–tritium plasma. The laser field is shown in green; blue arrows illustrate the magnetic field lines at the plasma interface; and red–yellow spheres are the laser-accelerated electrons that heat and ignite the fuel.



NIF PRESENCE AT SPIE OPTICS CONFERENCE

Plenary speakers at this year's SPIE Optics + Optoelectronics **conference**—held April 15–18 in Prague—included Ed Moses, Principal Associate Director for the National Ignition Facility (NIF) & Photon Science, who spoke on the status of NIF and future plans, such as NIF's transition to a user facility. In addition, NIF's Mike Dunne served as a symposium general chair at the conference, where more than 600 technical papers on the latest developments in optics and optoelectronic devices, technologies, and their integration were presented. A one-day workshop on laser energy included a discussion of the key enabling technologies and the underlying physics of laser-driven fusion and progress to "first ignition" at NIF.

NEW NUSTAR PHOTOS OF BLACK HOLES DEBUTED AT AAS MEETING

Among the new revelations unveiled at the American Astronomical Society's **Annual Meeting** in Long Beach were **NASA images** of previously unknown black holes newly detected with NASA's Nuclear Spectroscopic Telescope Array (NuSTAR). The x-ray-focusing optics for NuSTAR were developed at LLNL, where the technology dates back to the LDRD-supported High Energy Focusing Telescope (HEFT) instrument. The image below is of spiral galaxy IC 342, also known as Caldwell 5, with two black holes artificially colored based on data from NuSTAR. A **second image**, of supernova remnant Cassiopeia A, indicates where shock waves from the supernova blast are slamming into surrounding material, accelerating particles to nearly the speed of light. As the particles speed up, they give off a type of light known as synchrotron radiation. NuSTAR will be able to determine for the first time how energetic the particles are, and address the mystery of what causes them to reach such great speeds.

GEOSCIENTIST LEADS DEVELOPMENT OF DOE "ROADMAP" FOR ENHANCED GEOTHERMAL TECHNOLOGY

LLNL geoscientist John Ziagos led a team of DOE headquarters staff, researchers from other national laboratories, and program contractors in developing the DOE Geothermal Technologies Office (GTO) **document** *Technology Roadmap for Strategic Development of Enhanced Geothermal Systems (EGS)*. Development of the *Roadmap* began in the spring of 2011 at the request of the GTO Director. In August 2011, John organized and led a kickoff meeting in San Francisco, at which geothermal industry experts met to outline opportunities for advancing EGS technologies on 5- to 20-year timescales and come to agreement on the underlying technology needs. The *Roadmap* is based on this meeting and other input, summarizes the technology needs critical for commercializing EGS, and will guide priorities for future GTO investments in EGS.

RESEARCHERS FEATURED ON NEW DOE "WOMEN IN STEM" SITE

In conjunction with Women's History Month in March, DOE launched a new **website**—called "WOMEN @ ENERGY"—to feature women researchers and their work in the DOE complex, with the goal of demonstrating to young women who are considering a career in science, technology, engineering, or mathematics (STEM) the breadth of opportunities that are available in STEM fields at DOE's national laboratories and other sites. Among the many LLNL researchers profiled on the website so far are **Debra Callahan**, **Trish Damkroger**, **Maya Gokhale**, **Robin Goldstone**, **Kelley Herndon-Ford**, **Hye-Sook Park**, **Dawn Shaughnessy**, **Rea Simpson**, and **Eileen Vergino**.

NIF FEATURED IN "SCIENCE OF *STAR TREK*" DOCUMENTARY

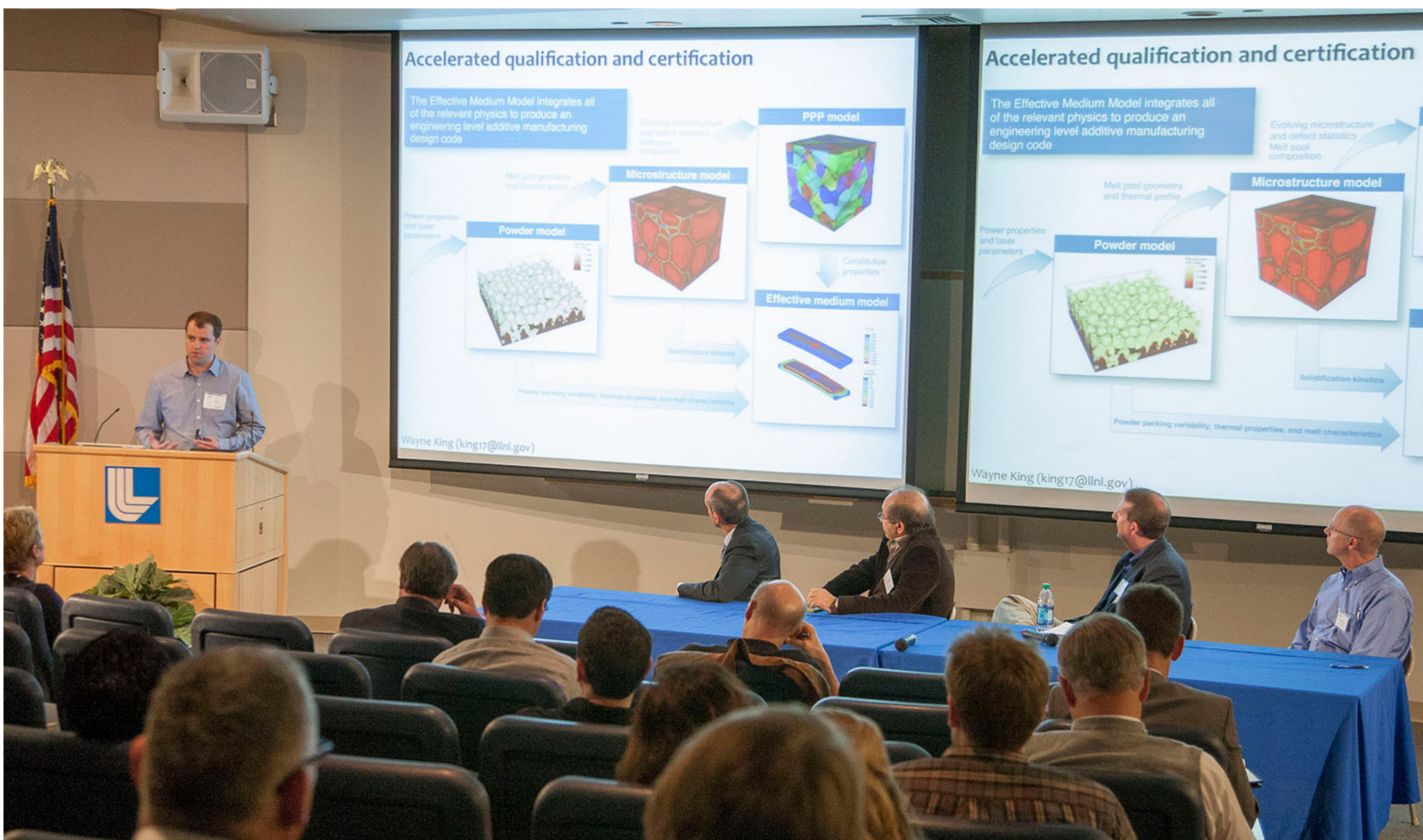
An 80-minute History Channel documentary titled *Star Trek: Secrets of the Universe* includes both a discussion of the possibilities of fusion energy as being investigated at NIF along with footage of the filming at NIF of scenes from *Star Trek Into Darkness*, in which NIF's target chamber is used as the fictional starship's warp core. The two screen captures from the documentary—**viewable online** in its entirety—show, right, the target chamber area during filming and, left, NIF and Photon Science PAD Ed Moses (right) presenting *Star Trek* director J. J. Abrams (center) with NIF's version of a dilithium crystal as actor Simon Pegg (to the left of Abrams) looks on.

LLNL Hosts Additive Manufacturing Forum

On March 20 at LLNL, the Laboratory **held a forum** on additive manufacturing for representatives of industry, other national labs, and government. The purpose of the one-day event was to inform manufacturers of the opportunities that additive manufacturing can provide their businesses and to highlight the importance of additive manufacturing to the national economy and to California. Keynote speakers were Scott Summitt, founder and Chief Technology Officer of Bespoke Innovations, and Kish Rajan, Director of the California Governor's Office of Business and Economic Development. The forum was sponsored by the Northern and Southern California Manufacturing Extension Partnerships, both of which are members of the newly formed California Network for Manufacturing Innovation, as are LLNL, Lawrence Berkeley Laboratory, i-GATE, NASA Ames Research Center, and the National Institute for Standards and Technology, among others. In the photo, LLNL engineer Eric Duoss gives a presentation as part of a **panel discussion** on innovation in additive manufacturing.

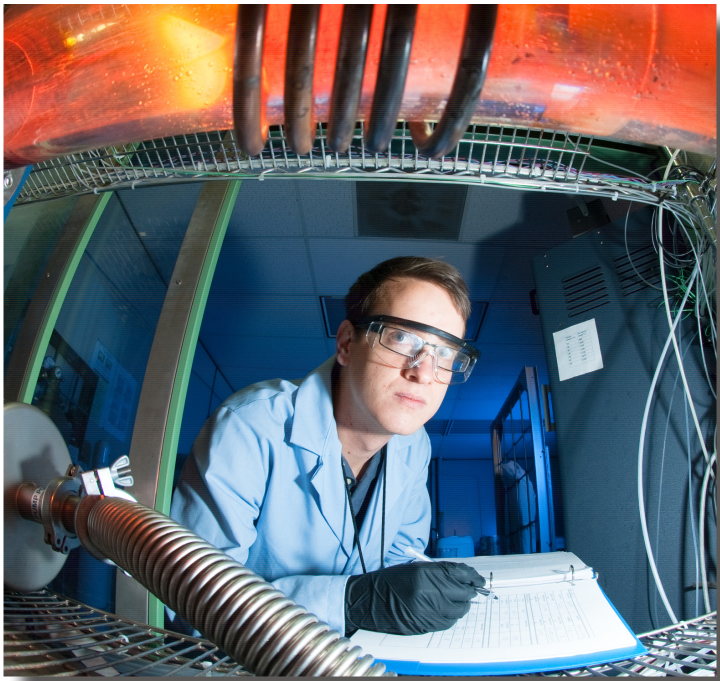
Bioprinter Work Profiled in *Wired*

Wired magazine recently **featured** LLNL genomics, bioinformatics, and computational biology researcher researcher Patrik D'haeseleer and his cutting-edge work on using 3-D bioprinters. "Instead of laboriously hand-placing cultures in a petri dish with a pipette," the article states, "researchers could prepare their experiments in software scripts, print out sheets of cells, and run experiments with the output—all on a postdoc's budget." Patrick demonstrates the printer in a **YouTube video**.



LAWRENCE SCHOLAR IS FIRST FROM KANSAS STATE

Kansas State University (KSU) doctoral student Clint Frye is one of 12 Lawrence Scholars chosen by LLNL this year—and the first ever from his university. As a scholar, Frye will spend 4 years conducting collaborative research at the laboratory and at the university—75 percent of his time researching at LLNL and 25 percent of his time performing related research on semiconductors at KSU. At LLNL, he is performing research with principal investigator Rebecca Nikolic on betavoltaics, which are devices that directly convert nuclear radiation to electrical energy. By coupling a semiconductor and a radioactive beta particle emitter, the researchers want to develop betavoltaic cells that can provide power for decades. “This is a researcher’s dream,” Clint said. “There are such great facilities and scientific expertise at Lawrence Livermore National Laboratory and I have access to so many resources, including scientists who are the best in their fields.” The Lawrence Scholar program “will enable me to do research that I might not be able to do anywhere in the country or the world,” he added. (Image courtesy of KSU.)



PUBLIC SERVICE AWARD FROM U.S. COAST GUARD

David Trombino, the LLNL representative on the Northern California Area Maritime Security Committee, received a certificate of appreciation from the U.S. Coast Guard on April 9 for his efforts in developing the Preventive Radiation and Nuclear Detection Program in the San Francisco Bay. David contributed to discussions to resolve issues involving shipping companies, facility and vessel security, law enforcement, and emergency management, and participated in numerous port security exercises. These efforts facilitated the adoption of the region’s “concept of operations” plan for preventive radiation and nuclear detection, placing San Francisco Bay Area law enforcement agencies among the first in the nation to use radiological source detection equipment for routine operations. The Northern California Area Maritime Security Committee is charged with helping coordinate, plan, share information, and conducting other necessary activities to aid the security of the Marine Transportation System within the Port of San Francisco’s area of responsibility. In the photo with David is U.S. Coast Guard Captain Cynthia Stowe, commander of the Coast Guard’s San Francisco sector.

CLIMATE SCIENTIST SPEAKS AT NATIONAL CLIMATE ASSESSMENT FORUM

Lab climate scientist Philip Duffy (far left in the photo) was one of five scientists whose work contributed to the findings of the National Climate Assessment (NCA) draft report and who spoke **at a forum** hosted by the University of Southern California (USC) Price School of Public Policy on April 8. The forum explored the impacts projected to result from climate change and was kicked off by former California Governor Arnold Schwarzenegger, who said, “The National Climate Assessment is our physical. These scientists have done thorough research, and they can tell us our condition and give us a prescription for what we need to do to improve the health of our climate.” Philip, in his talk, explained that although the report uses many different climate models to improve accuracy, some uncertainty in climate projections is inevitable because one cannot exactly predict future production of greenhouse gases, natural variability, or every detail of the climate system’s response to greenhouse gases. Some of the findings from the NCA’s Southwest Region Chapter—which is **available online**—include projections that sea levels will rise between 1 and 1.4 meters by the year 2100, putting 480,000 people and nearly $100 billion in property along the California coast in jeopardy, and that stream flow in the Sacramento–San Joaquin River Delta, the Colorado, the Rio Grande, and the Great Basin were 5 to 37 percent lower between 2001 and 2010 than the 20th century averages. (Photo courtesy of USC/Tom Queally.)

LLNL CONTRIBUTES TO LATEST HIGGS BOSON FINDINGS

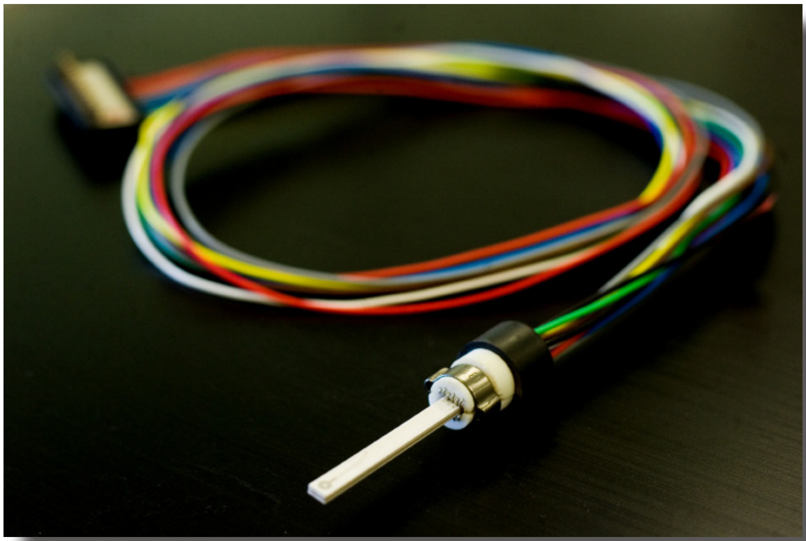
Laboratory scientists played a role in the latest results announced by CERN that provide further evidence that the subatomic particle discovered last year is the elusive Higgs boson, a particle at the heart of the Standard Model of particle physics. The new evidence resulted from the analysis of additional data from the A Toroidal LHC Apparatus (ATLAS) and Compact Muon Solenoid (CMS) collaborations at the Large Hadron Collider (LHC)—data that were not yet available at the time of the July 2012 announcement of the particle’s discovery. ATLAS and CMS are detectors for recording and measuring particle collisions inside the LHC, the world’s largest and most powerful particle accelerator. “These new results are pretty impressive, adding not just more statistics, but new information showing that we have a Higgs boson,” said Livermore’s Doug Wright, who leads LLNL’s CMS team. “Ultimately this will tell us something about the evolution of the universe and perhaps a clue towards a Grand Unified Theory.” Researchers unveiled the new evidence at the Rencontres de Moriond **conference** in La Thuile, Italy on March 7.

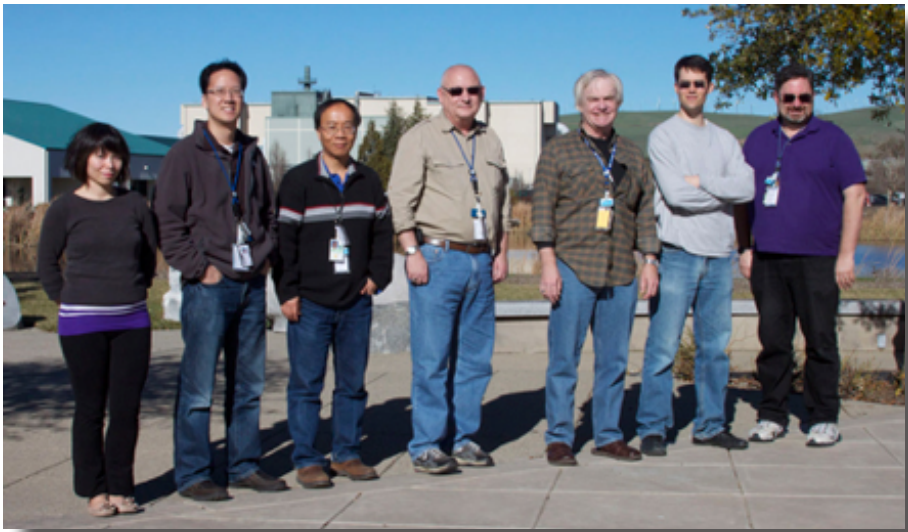
TEAM HELPS BUILD SOFTWARE TOOLS FOR WHITE HOUSE CARBON CAPTURE INITIATIVE

A team of Computation and Engineering staff contributed to the first release last fall of software tools for the Carbon Capture Simulation Initiative (**CCSI**). The software—released a year ahead of schedule—includes uncertainty quantification (UQ) tools, carbon capture simulation models, risk analysis tools, a reduced-order model-development tool, and the Turbine Gateway, which allows thousands of UQ simulations to run simultaneously on the Amazon EC2 cloud. DOE Deputy Assistant Secretary for Clean Coal **James Wood** commended the quality of the initial software release, saying, "The usefulness of the tools was demonstrated in a breakout session [at the CCSI Industry Advisory Board meeting] during which industry representatives began to voice plans for immediate use of these tools. Success in [this] goal has significant uses in many industries that use complex systems and offers a potential to reduce costs, risks, and the enormous time lag presently required to bring commercial products to market." DOE launched CCSI to meet a White House **task force**'s goal to overcome the barriers to widespread, cost-effective deployment of carbon capture technology within 10 years. In the photos are (left to right) LLNL team members Brenda Ng, Jeremy Ou, Charles Tong, Bill Oliver, Greg Pope, Jim Leek, and Top Epperly.

COMMERCIALIZATION OF NOx SENSOR MARCHES ON

Emisense, which has a cooperative R&D agreement with LLNL to develop Livermore NOx sensor technology, recently closed its third round of funding in this ongoing enterprise. In addition, Emisense has partnered with CoorsTek in support of this commercial sensor development. This recent advance follows on the heels of the company making multiple crucial development milestones for the NOxTrac and other sensor technologies in 2012. As demonstrated by these latest advancements, Emisense continues to translate LLNL NOx technology into specific, practical, manufacturable product designs.





LLNL Attends "IP State of the Union"

Business development executive Ida Shum and other representatives from LLNL attended this year's IP100 Executive Forum, a closed-door **summit** that provides a "rare opportunity for top decision makers and thought leaders to discuss pivotal IP business issues and strategies for boosting innovation." This year's event was attended by an array of corporate giants, including Google, Bayer, Eli Lilly, Merck, Microsoft, and Schlumberger. Cheryl Martin, Deputy Director for Commercialization for DOE's **ARPA–E**, spoke about the agency's work to catalyze and support high-potential energy technologies through funding and technical assistance during the early stages of innovation. Commented Kirk Dailey, head of patent transactions for Google, "This event is like an annual 'IP State of the Union,' with a hundred or so of the business world's best and brightest. I attended because I wanted to be part of the dialogue, and I'm certainly glad I did."

Climate Scientist Among International Attendees at Conference

Livermore climate scientist Ben Santer was among the scientists and policymakers from around the world who gathered March 20–22 at the University of California, Davis, to grapple with the threats of climate change for global agriculture and to recommend science-based actions to slow its effects while meeting the world's need for food, livelihood, and sustainability. The Climate-Smart Agriculture: Global Science **Conference**, planned in coordination with the World Bank, builds on a 2011 international meeting on this theme in the Netherlands. The conference considered the implications of cutting-edge agricultural, ecological, and environmental research for improved design of policies and actions affecting agricultural management and development; identified farm and food-system issues; determined research gaps; highlighted emerging research initiatives; and studied transformative policies and institutions.

Letter of Intent for Proton Therapy

Compact Particle Acceleration Corp. (CPAC), a company created as an offshoot of Madison-based TomoTherapy, reported in November it had received a letter of intent for one of the first proton therapy systems from **Southwest Oncology Centers**. The company's technology is based on LLNL's dielectric wall accelerator technology. Proton therapy is considered a more advanced radiation treatment system for cancer patients, but a problem with the relatively few existing proton therapy centers is that they require property the size of a football field and can cost $150 million to $200 million. CPAC, now based at Livermore, **has designed a system** to be far, far smaller and much less costly.

Researcher to Co-Chair Workshop on Sustainable Bioenergy

Jennifer Pett-Ridge has been asked to be one of three co-chairs of a DOE Office of Biological and Environmental Research Workshop on Research for Sustainable Bioenergy, planned for October 2013 in the Washington, D.C. area. Jennifer will organize aspects of the workshop relevant to root-zone microbial processes. Co-chairs Phil Robertson of Michigan State University and Michael Udvardi of the S.R. Noble Foundation will cover sustainability and plant feedstock genomics, respectively. The goals of the workshop are to better understand the interconnections between sustainable bioenergy feedstocks and ecosystem services, identify how these gaps can be addressed using the tools of systems biology and genomics, and identify paths for developing models that can accurately predict the impact of plants, microbes, and environmental attributes on the sustainability of feedstock production and ecosystem services at appropriate geographic scales.

LLNL Plays Major Role in X-Ray Optics Workshop

The DOE Office of Basic Energy Sciences (BES) held the DOE Workshop in X-ray Optics for BES Light Source Facilities on March 27–29. This invitation-only workshop "assess[ed] the state of the art and future development requirements, with emphasis on the underlying engineering, science, and technology necessary to realize the next generation of x-ray optics instruments." The workshop's deliverable will be a report that summarizes the workshop activities and lists prioritized research directions to address key challenges. Livermore researchers co-chaired three of 11 topic areas, making LLNL the only national laboratory that does not operate an x-ray light-source to have staff chairing any of the sessions. The Laboratory's participation and prominence in this workshop results from a recognition of the Lab's capabilities and expertise in x-ray optics and x-ray–matter interactions, and a concerted effort over the last several years by LLNL, and Michael Pivovaroff in particular, to be an active partner with the four DOE National Laboratories that do operate x-ray light sources as user facilities for BES. The LLNL participants include Stefan Hau-Riege (participating expert on photon–matter interaction), Michael (co-chair of a session on models for optics facility operation and R&D), Lisa Poyneer (co-chair of the adaptive optics session), and Regina Soufli (co-chair of the thin films session).

Ten Years On, LLNL Software Still Running on World's Fastest Supercomputers

Originally developed at LLNL 10 years ago and subsequently commercialized, Slurm Workload Manager today is the **most widely used** such software on the world's fastest supercomputers—running on 33% of the 15 fastest on the TOP500 list, as of late last year.

New Initiative Funded to Improve Lithium-Ion Battery Technology

A multilab team including LLNL's Vincenzo Lordi, Erik Draeger, and Mitchell Ong recently received a 5-year, $3.7 million grant from DOE Basic Energy Sciences and Advanced Scientific Computing Research Programs, through the Scientific Discovery through Advanced Computing Program, to conduct research to understand key aspects of the chemistry and dynamics of lithium-ion batteries, particularly at interfaces. For instance, no comprehensive theoretical understanding currently exists about the formation and evolution of the solid–electrolyte interface layer, which has hindered progress in designing optimal electrolyte–anode systems. Using Sequoia and other supercomputers at LLNL and LBNL, the team will combine state-of-the-art quantum mechanical methods to reach the length and time scales required to capture the essential dynamics of these complex, multiphase lithium-ion systems. "In so doing," said lead scientist John Pask of LLNL, "we aim to achieve a breakthrough in the understanding of these ubiquitous electrochemical systems, and thereby pave the way for fundamental advances in these central technologies."

Rad Material Detector Technology Licensed

The Laboratory signed a license agreement with AMETEK Advanced Measurement Technology for an LLNL technology titled "Hand-Held, Mechanically-Cooled, Radiation Detection System for Gamma-Ray Spectroscopy." AMETEK, a large business located in Oak Ridge, TN, is a leading global manufacturer of electronic instruments and electric motors. The company plans to use this technology for the purpose of developing and commercializing a new instrument to detect radiation materials.

DTEM-Enabled Phase Plate Technology Licensed

In April, the Laboratory signed a limited exclusive patent license with Integrated Dynamic Electron Solutions for a technology titled "Pulsed Ponderomotive Phase Plate, Co Lens, and Movie Mode." The Belmont, CA–based startup producing analytical instruments will use the technology in electron optical devices. This phase plate technology is one result of LLNL's research in understanding rapid material dynamics in extreme conditions utilizing the Laboratory's dynamic transmission electron microscope (DTEM). DTEM has won an **R&D 100**, a Nano50, and a Microscopy Today Innovation **award**.

Combat Simulator Installed for Australian Military

LLNL's Conflict Simulation Laboratory completed the installation and user training of JCATS and JLOD for 25 military personnel and contractors at the Australian Joint Combined Training Capability Center. JCATS (Joint Conflict and Tactical Simulation) is an interactive, effects-based simulation for training, planning, and rehearsing tactics, and for analyzing resource deployment, weapon effectiveness, and force structures. JLOD (JCATS Low-Overhead Driver) is a simulation model used to fill exercise gaps, such as modeling civilian clutter, commercial shipping lanes, and detailed emission signatures for large entity counts of various types of radars. Training at the Australian Joint Combined Training Capability Center was provided by Computation's Joe Wilson, Andy Pomykal, and Abel Gezahegne, and Engineering's Will Belue and Jim Barnett. The newly trained personnel will use JCATS in a brigade-level rehearsal this month in preparation for a major training event later this year.

Lab Partners in Groundbreaking Biosolids-to-Energy Project

LLNL has partnered with Miami, FL–based Chemergy, Inc. to develop and demonstrate an innovative bioenergy technology for converting biosolids to energy efficiently. Once developed, the new technology will be demonstrated at the Delta Diablo Sanitation District facility in Antioch, CA, under the sponsorship of Bay Area Biosolids to Energy (**BAB2E**)—a consortium of 19 San Francisco Bay Area public agencies responsible for wastewater treatment—with funding from the California Energy Commission and private investment. The LLNL–Chemergy, Inc. technology will convert wet biosolids into hydrogen for use in generating electricity using fuel cells, which in the demonstration will be contributed by the Department of Defense. The process involves aqueous chemical processing at moderate temperature and will allow much higher feedstock use than competitive processes, such as anaerobic digestion or fermentation, while also avoiding the need for the capital-intensive equipment used in high-temperature gasification or pyrolysis. The project is expected to serve as a model for other U.S. metropolitan areas. LLNL scientist Robert Glass will serve as principal investigator of the LLNL portion of the project.

CRADA with Johns Hopkins for Dislocation Dynamics Code

The Laboratory signed a cooperative research and development agreement (CRADA) in April with Johns Hopkins University to develop technology for predicting the behavior of magnesium polycrystalline alloys undergoing dynamic deformation. Under the CRADA, Livermore will leverage its **ParaDiS** dislocation dynamics code with finite element coupling. Up to now, the ParaDiS code has been restricted to periodic or infinite domains.

GRANT FOR RESEARCH ON CLIMATE–MARINE MICROBIOLOGY LINK

Xavier Mayali has received a grant of nearly $1 million from the Gordon and Betty Moore Foundation's Marine Microbiology Initiative to study how the food preferences of coastal marine microorganisms shape elemental cycles in the ocean. The Foundation's grant, which will be administered through Oregon State University (OSU), will allow Xavier and LLNL colleague Jennifer Pett-Ridge, along with coinvestigators at OSU and Oak Ridge National Laboratory (ORNL), develop a deeper understanding of how the food choices of marine microbes contribute to carbon cycling off of the coast of California. High-precision isotopic techniques and molecular biology methods that are being pioneered at LLNL and ORNL will be used to identify which microbes prefer which general types of organic molecules (e.g., lipids, carbohydrates, proteins, and nucleic acids) and how microbial food-web interactions affect the marine carbon cycle. Developing a better understanding of how the marine biosphere will respond to increasing levels of atmospheric CO_2 is vitally important for reducing uncertainty in climate model predictions.

PAPER ON MARS SCIENCE LABORATORY PREPARATIONS PRESENTED AT ANS CONFERENCE

Researcher Ron Baskett presented a **report** titled *Technological Advances in Radiological Contingency Planning for the 2011 Mars Science Laboratory (MSL) Mission* at the American Nuclear Society **conference** Nuclear and Emerging Technologies for Space. Coauthored with LLNL colleague Steven Homann and NASA and DOE Office of Nuclear Energy teammates, the paper summarized 5 years of coordination across more than two dozen local, state, and Federal agencies to develop state-of-the-science response capabilities for the unlikely event of an accidental atmospheric release of radiological material contained in the MSL's radioisotope thermoelectric generator. LLNL fulfilled two key roles: (1) serving as senior science advisor, including providing support with Livermore's National Atmospheric Release Advisory Center; and (2) leading the effort to develop and implement a fully automated network of monitors that provided real-time alpha air concentration measurements downwind of the launch site and in surrounding communities. NASA has employed radioisotope thermoelectric generator for five decades without any untoward consequences, and MSL was no exception.

BEAM-SIMULATION CODE GOES OPEN SOURCE

WARP, originally developed to simulate space-charge-dominated ion beams in accelerators for the Heavy Ion Fusion Virtual National Laboratory, has recently been granted open-source status after DOE's Office of Fusion Energy Sciences concluded that the needs of its growing user community could best be met if the code could be used without restriction by scientists across the U.S. and worldwide. Researchers in LLNL's Fusion Energy Sciences Program have been the principal developers of WARP, with major contributions from LBNL. Recently highlights of WARP's use include playing a major role in the physics design of the NDCX-II ion accelerator at LBNL, but the code has also found a broad range of other applications, including non-neutral plasmas in traps, stray electron clouds in accelerators, laser-based acceleration, muon cooling, coherent synchrotron radiation, and the capture and focusing of ion beams produced by short-pulse-laser-irradiated foil targets.

LLNL TECHNOLOGIES OPTIONED BY SMALL BUSINESSES

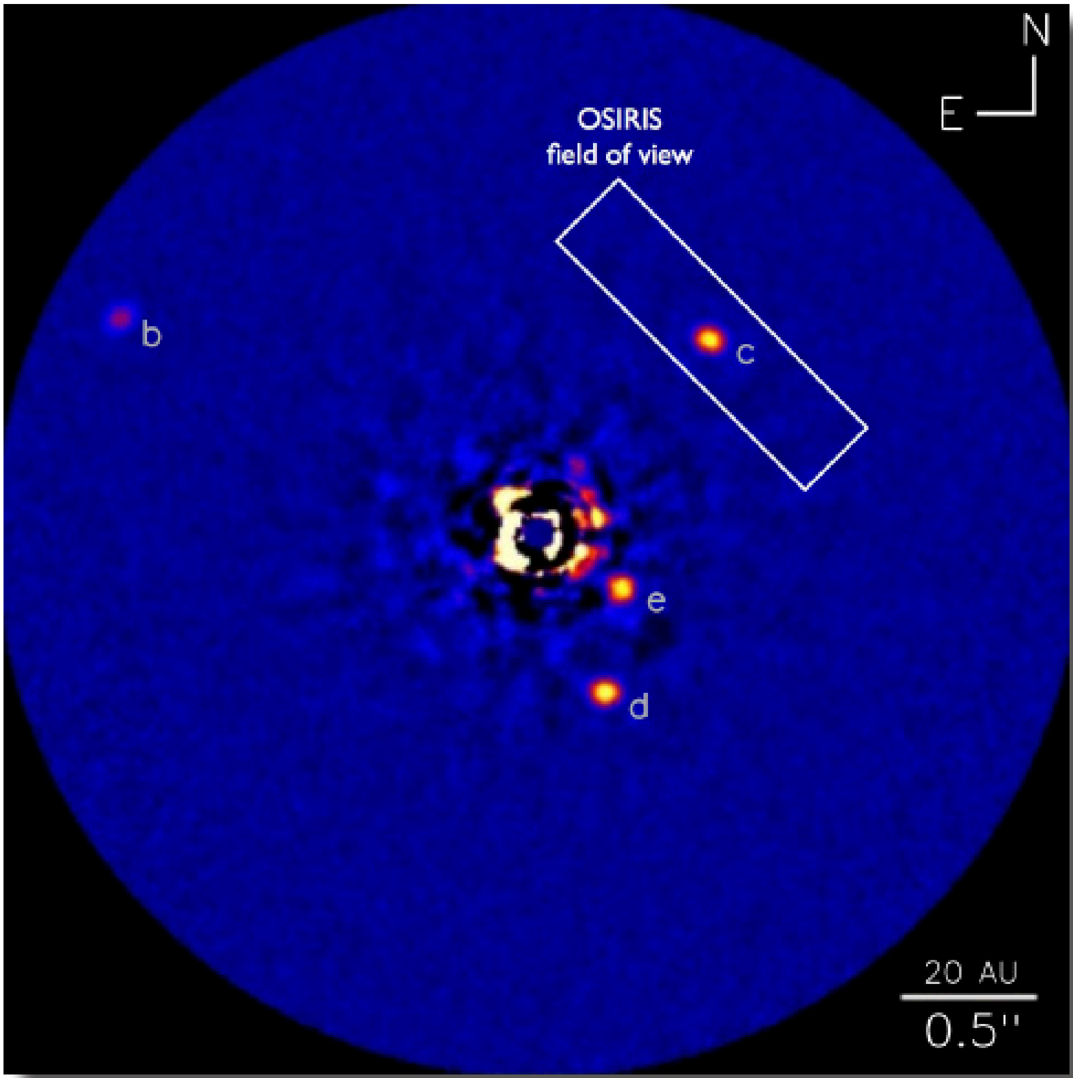
Aeneid Technologies optioned two LLNL technologies in April. One, titled "Electrostatic Generator Technology for Electrostatic Generators/Motors for Power Generation and Prime Mover Motor Applications at Speeds up to 600 RPM," has possible applications in power generation and prime mover applications. The other technology is titled "Electromechanical Battery Technology for Flywheel-Generator Modules for Energy Storage Applications Under 200 kWH," applications of which the company will investigate for flywheel-generator modules for energy storage applications. Aeneid Technologies is a startup located in Moraga, CA. In addition, Vancouver, WA-based Malignext Target Technologies optioned the technology "Disposable Sexually Transmitted Diseases (STD) Panel Detector" for possible use in detecting STDs. Malignext Target Technologies is also in the research phase of developing a product that will be able to mark or make palpable lesions or tumors of the breast.

RESEARCHER NAMED ASSOCIATE EDITOR OF JOURNAL, RE-ELECTED TO RADIATION BOARD

Annie Kersting, Director of the LLNL branch of the Glenn T. Seaborg Institute, has been asked to serve as associate editor of *Geochimica et Cosmochimica Acta*, the official journal of the Geochemical Society and the Meteoritical Society. The journal publishes original research and reviews spanning a wide range of subjects in terrestrial geochemistry, meteoritics, and planetary geochemistry, including the physical chemistry of gases, aqueous solutions, glasses, and crystalline solids; igneous and metamorphic petrology; chemical processes in Earth's atmosphere, hydrosphere, biosphere, and lithosphere; and isotope and planetary geochemistry. Annie was also reappointed to the National Academy of Sciences' Nuclear Radiation & Studies Board (NRSB) for a 2-year term through 2014, after having been appointed in 2010 for a 3-year term. The NRSB organizes and oversees studies on safety, security, technical efficacy, and other policy and societal issues arising from the application of nuclear and radiation-based technologies, including exposure to ionizing and non-ionizing radiation; malevolent uses of nuclear and radiation-based technologies; and the risks, benefits, and efficacies of nuclear- and radiation-based applications in medicine and other fields.

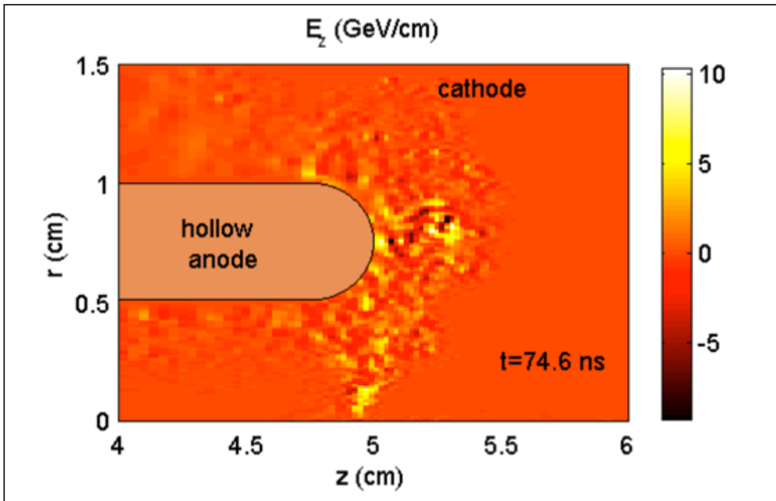
SCIENCE PAPER ON MOST-DETAILED EXOPLANET ATMOSPHERE SPECTRUM

LLNL astronomer Bruce Macintosh, working with a team of international scientists, has made the most detailed examination yet of the atmosphere of a Jupiter-like planet beyond our solar system. The finding provides additional insight into how planets are formed. A **paper announced these results** in *Science*, which also **featured** the work in a "Perspectives" piece. The team, using the OSIRIS instrument on the Keck II telescope on the summit of Mauna Kea, Hawaii, uncovered the chemical fingerprints of specific molecules, revealing a cloudy atmosphere containing water vapor and carbon monoxide. The unprecedented level of detail was made possible by Keck Observatory's advanced instrumentation and by groundbreaking observing and data-processing techniques. "This is the sharpest spectrum ever obtained of an extrasolar planet," said Bruce. "This shows the power of directly imaging a planetary system—the exquisite resolution afforded by these new observations has allowed us to really begin to probe planet formation." The figure is one of the discovery images obtained at Keck II using the adaptive optics system and NIRC2 Near-Infrared Imager, with the rectangle indicating the field-of-view of the OSIRIS instrument for planet C.



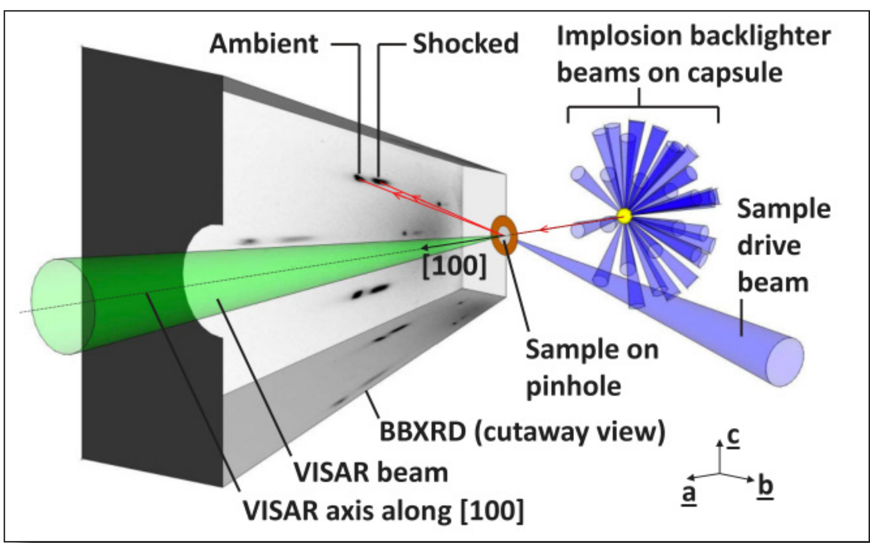
RESEARCHERS DEVELOP FIRST KINETIC MODEL OF PLASMA FOCUS DEVICE

Livermore scientists Andrea Schmidt and Vincent Tang describe, **in a paper** in *Physical Review Letters*, their first-ever demonstration of a fully kinetic model of the dense plasma focus Z-pinch device in a realistic geometry. The new simulations have reproduced key features of Z-pinch plasmas, including the ion beam and neutron outputs, and produced signatures of a type of instability that has always been postulated to fundamentally drive the dynamics in these plasmas. Their simulations also reproduce experimental neutron yields and high-energy beams for the first time. This simulation tool will be used to further unravel the unknowns of this age-old plasma configuration. Says Andrea: "We now have, for the first time, demonstrated a capability to model these plasmas fully kinetically, allowing us to simulate the pinch process at the particle scale." The figure depicts the E_Z field inside the fully kinetic simulation in the middle of the pinch, which is located near $r = 0$ cm.



RECORD-SETTING IN SITU X-RAY DIFFRACTION ALSO VALIDATES LIVERMORE MODEL

A group of researchers from LLNL and the United Kingdom's Atomic Weapons Establishment and Oxford University have **published a paper** in *Physical Review Letters* in which they describe compressing samples of tantalum (Ta) to shock pressures of 0.6 to 2 Mbar using in situ x-ray diffraction—the highest pressure to which the technique has ever been used to shock-load a high-atomic-number metal. The experimental geometry directed some light from the Omega laser to a backlighter capsule, generating x-rays that passed through the Ta sample and created a Laue x-ray diffraction pattern that was recorded; changes in the diffraction pattern during compression reflect the deformation of the crystal lattice. The results of the experiments also showed that various models—with the exception of a multiscale strength model developed at LLNL—underpredicted the strength as measured in the experiment. The figure shows the experimental geometry, including the broadband x-ray diffraction (BBXRD) diagnostic and the LLNL-developed Velocity Interferometer System for Any Reflector (VISAR). Some of the work done at Livermore was supported by LDRD.

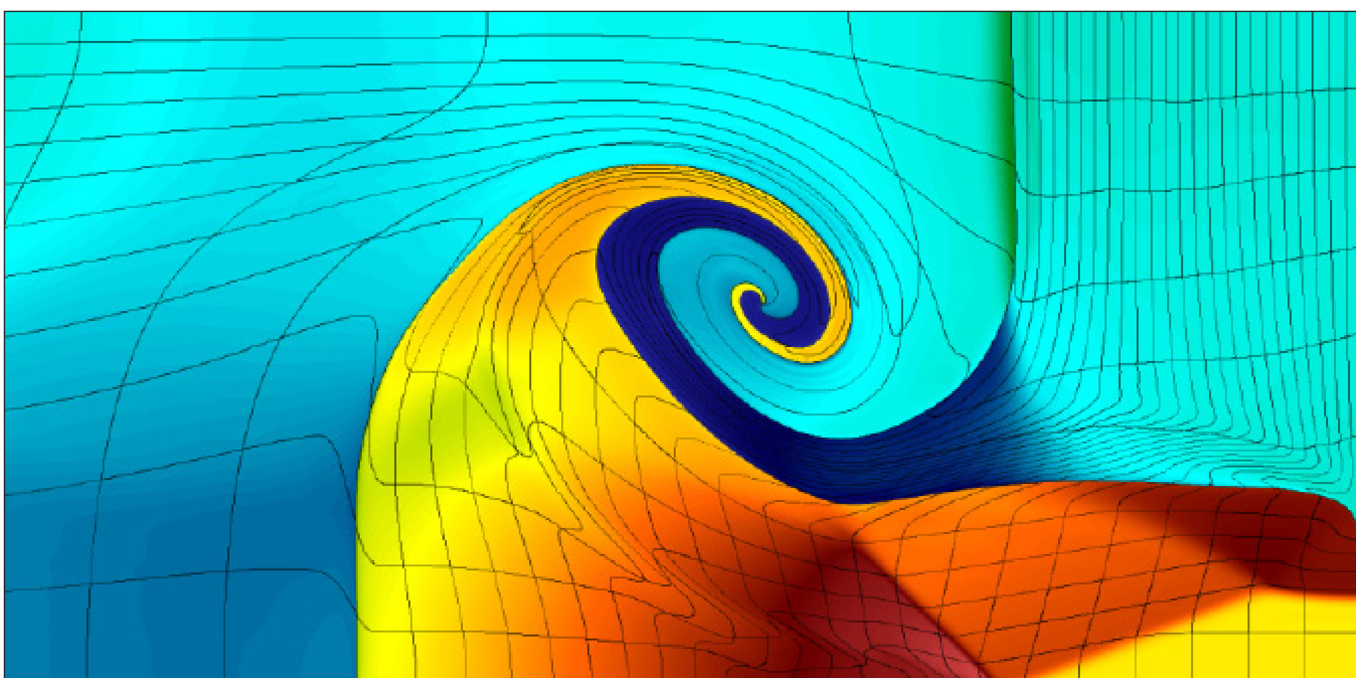


BLAST Code Ready for Extreme Parallelism and Exascale

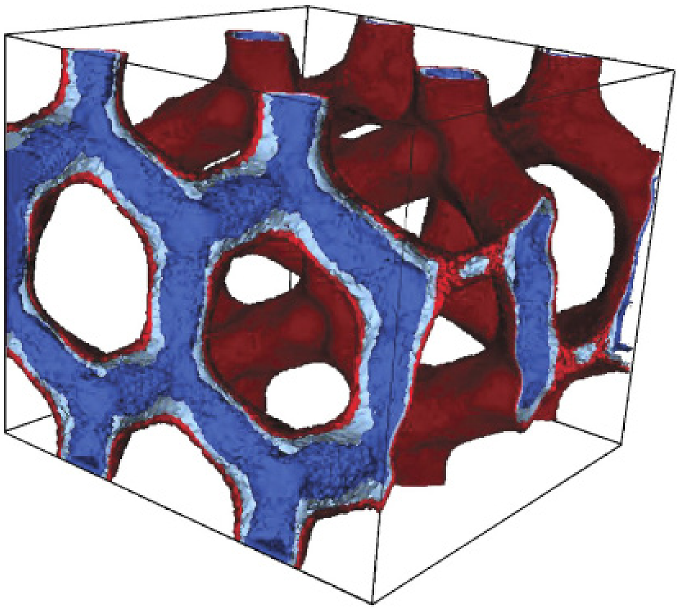
Researchers at Lawrence Livermore have developed **BLAST**, a high-order finite-element hydrodynamics research code that improves the accuracy of simulations and provides a viable path to exascale architectures and extreme parallel computing, such as Livermore's own Sequoia, which has over 1.5 million cores. The figure shows a very high-order calculation of a multimaterial shock hydrodynamics problem using Q_7–Q_8 finite elements (eighth-order polynomials for the kinematic fields, seventh-order polynomials for the thermodynamic fields). The high-order finite elements result in highly curved zones and subzonal resolution of the shock waves, which is simply not possible with a low-order method. As a high-order method with a greater flop/byte ratio, BLAST also provides a high-performance computing advantage in that more time is spent on floating-point operations relative to memory transfer, an important parameter for exascale computing. BLAST also enables excellent scaling, down to very few computational zones per processor. "I don't know of any other code that has such good strong scaling," said BLAST principal investigator Tzanio Kolev. "And I think we can push it even further."

LLNL Paper Among Most-Downloaded in 2012 from *Plasma Physics and Controlled Fusion*

A **paper** by Bick Hooper and colleagues on LLNL's Sustained Spheromak Physics Experiment (**SSPX**) has been acknowledged by the journal *Plasma Physics and Controlled Fusion* as one of the 20 most downloaded articles last year and has also been selected as a **highlight of 2012**. The paper describes the design and results of SSPX to study spheromak physics with a focus on sustained, long-pulse operation and the possibility of achieving steady-state or quasi-steady-state operation with good energy confinement. The paper concludes that "the buildup and current sustainment by coaxial helicity injection in SSPX degraded thermal confinement by opening the magnetic surfaces during its application, but successfully generated high-quality plasmas used in confinement and other physics studies." In this work, LLNL collaborated with UC San Diego, the University of Maryland, University of Wisconsin, and Seattle-based Wodruff Scientific, Inc.



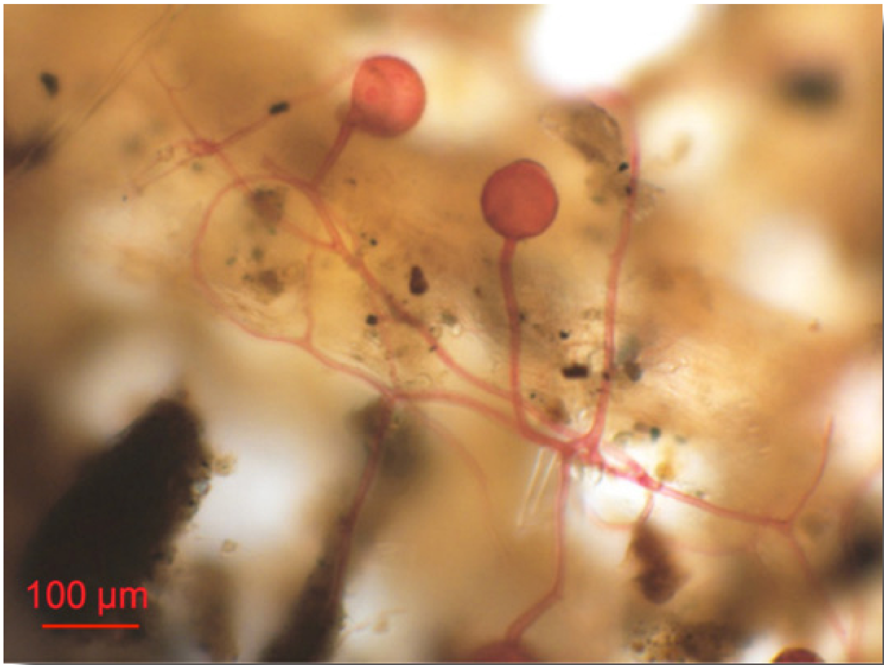
NEW METHANE-CAPTURING MATERIAL ANNOUNCED



A **paper published** in *Nature Communications* announces the joint discovery by LLNL and UC Berkeley of new materials that capture methane, a powerful greenhouse gas. "Methane capture poses a challenge that can only be addressed through extensive material screening and ingenious molecular-level designs," said LLNL co-author Amitesh Maiti (whose work on methane capture was also **recently featured** in *Scientific American*). The LLNL–Berkeley team performed systematic computational screening, including roughly 100,000 zeolite structures, uncovering a few nanoporous candidates that appear promising. In the team's simulations, one specific zeolite, dubbed SBN, captured enough medium-source methane to turn it to high-purity methane, which in turn could be used to generate efficient electricity. Work at LLNL was funded by the Advanced Research Projects Agency-Energy. The figure shows a unit cell of SBN with the low-energy strong binding sites for methane highlighted dark blue.

PLANT-FUNGUS SYMBIOSIS SHOWN TO PLAY ROLE IN CARBON AND NITROGEN CYCLING

A recent *Environmental Microbiology* **paper** by a UC Berkeley graduate student, LLNL's Jennifer Pett-Ridge and Peter Weber, and colleagues at UC Berkeley and the U.K.'s University of York reports on studies of carbon and nitrogen transfer between plants and arbuscular micorrhizal fungi (AMF) and the effects of AMF on the makeup of the soil microbial community. (The work was also featured on DOE Genomic Sciences Program website.) AMF form symbiotic affiliations with the roots of many plants, but the details of this relationship have remained poorly understood. The research used "omics" tools combined with LLNL's nanoscale secondary ion mass spectrometry of isotopically labeled compounds to unravel the interactions of AMF, plant roots, and soil microbial communities. The authors found that AMF increase the abundance of plant-litter-degrading microbes, which liberate nitrogen-containing compounds from dead plant matter. This nitrogen is taken up and transferred by the AMF to their host plants. These findings provide important insights into the complex routes by which carbon and nitrogen flow through ecosystems. The figure shows AMF hyphae with spores growing in decomposing litter.

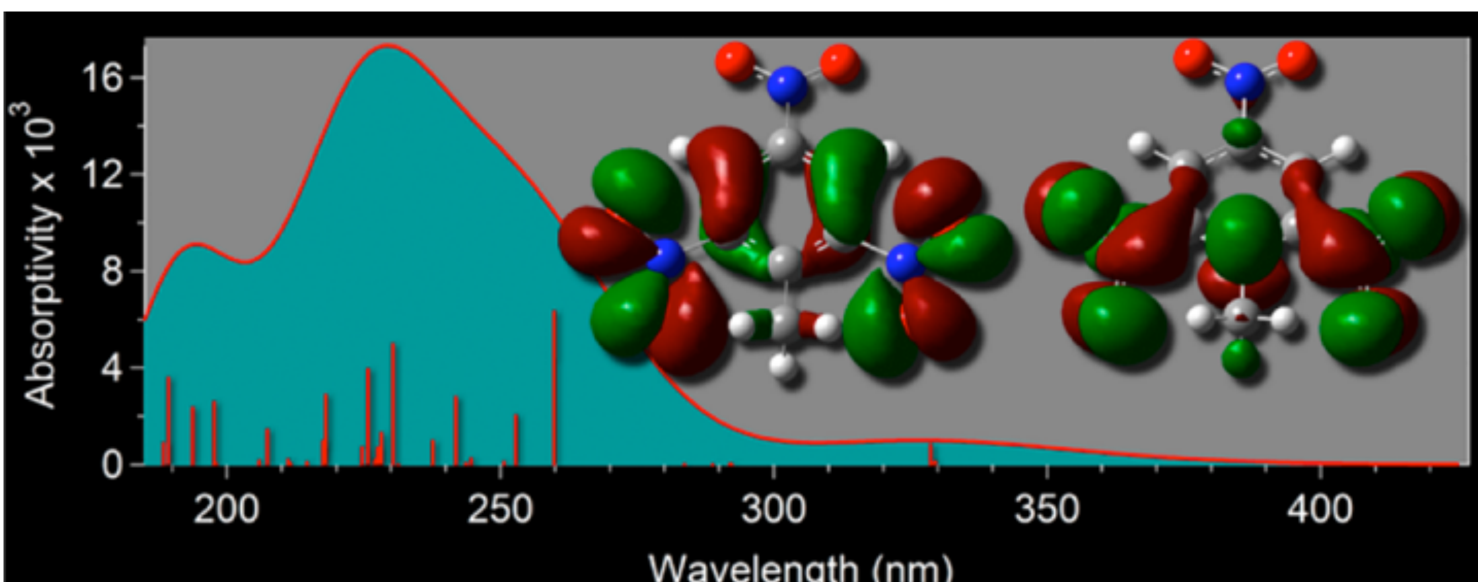


EXPERIMENTAL–THEORETICAL OPTICAL ABSORPTION STUDY OF EXPLOSIVE MOLECULES

Laboratory chemist Christian Grant and colleagues from UC Santa Cruz **have published**—in the online edition of the *Journal of Physical Chemistry A*—an article on a combined experimental and theoretical study of the optical absorption of six common explosive molecules. Time-dependent density functional theory (TD-DFT) was used to calculate the excitation energies and oscillator strengths of the explosives, and the results were compared to experimental ultraviolet–visible absorption spectra collected in acetonitrile. For each molecule studied, the natural transition orbitals were reported for the most prominent singlet excitations. The TD-DFT results were combined with the ionization potentials to construct energy level diagrams for the six compounds. These results can be used to guide development of approaches for fluorescence-based detection methods for these explosives. The figure shows the predicted absorption transition energies and absorption spectrum for TNT obtained by TD-DFT computations. The ground (left) and excited state (right) natural transition orbitals are shown for the electronic transition occurring at 329 nm.

BREAKTHROUGH COULD MAKE HIGH-FIDELITY "DEEP SEQUENCING" A REALITY

In a **paper published** in the online edition of *BMC Genomics*, LLNL researchers Haiyin Chen-Harris, Monica Borucki, Clinton Torres, Tom Slezak, and Jonathan Allen describe a new technique that significantly reduces error rates in deep genetic sequencing—that is, sequencing that provides multiple independent "reads" of a given portion of a genome—and improves the detection accuracy for rare variants. Using their new sequencing protocol and an error model optimized for variant detection, they were able to characterize a large number of genetic mutations present in a viral population at ultralow frequencies. Such improvements in deep sequencing could overcome a current limitation—the difficulty in differentiating real, low-frequency mutations from sequencing errors—and enable the approach to live up to its potential to accurately determine the full spectrum of genetic mutations in a population and examine the dynamics of mutations in detail. In addition to viral evolution, the new rare-variant detection strategy of Haiyin et al. could also be applied to any basic or clinical research area that requires the identification of rare mutations.

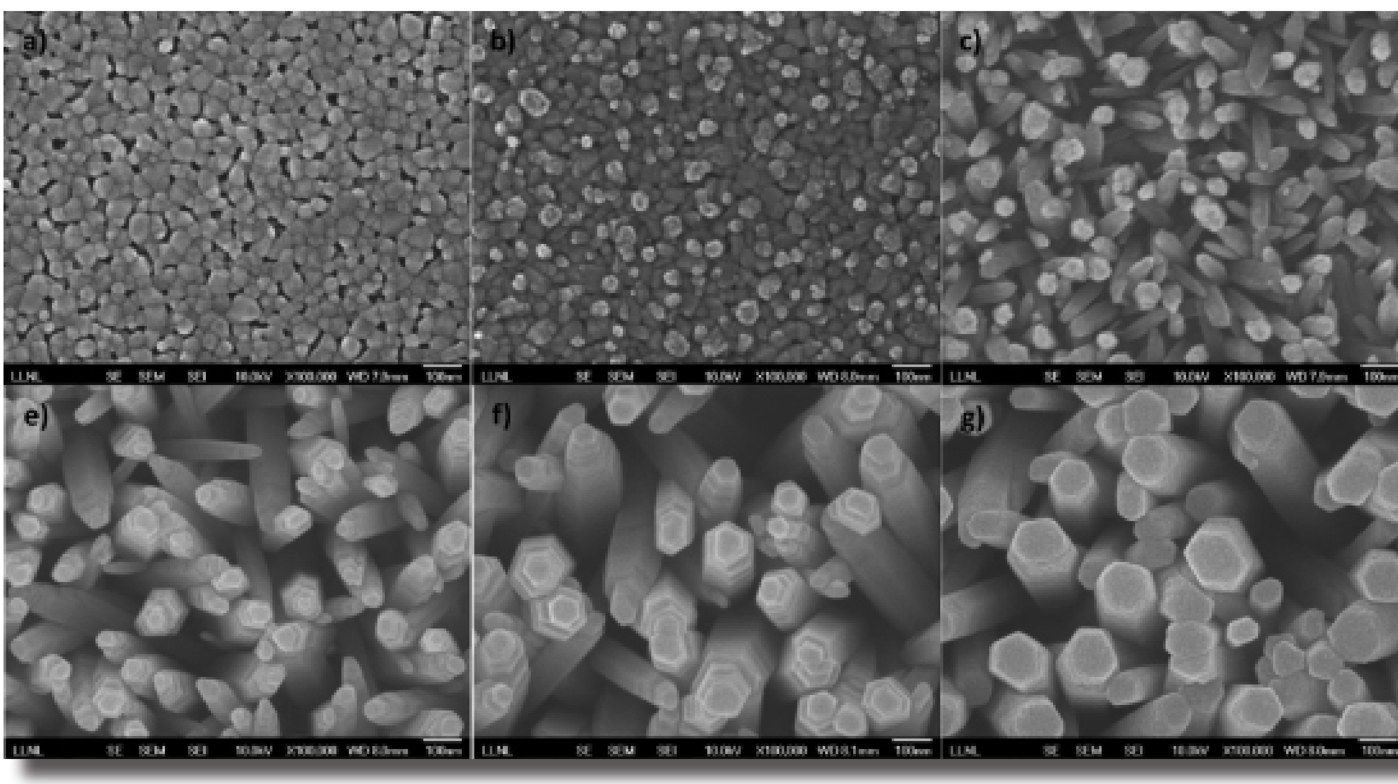


FIRST-EVER TEST OF NANOWIRE GROWTH MODEL PUBLISHED

In a special issue of *Chemistry of Materials* dedicated to synthetic and mechanistic advances in nanocrystal growth, Lab researchers Tammy Olson, Alexander Chernov, Joe Satcher, and Yong Han and U.S. Air Force Academy colleague Brent Drabek report **their experimental validation** of the geometrical selection model for hydrothermally grown zinc oxide (ZnO), which has potential applications in solar cells, lasers, photocatalysis, waveguides, and photodetectors, leading to considerable interest in understanding how to optimize the growth of ZnO structures. The paper by Tammy et al. reports the first-ever experimental test of the geometric selection model as applied to nanowires. Comparing the results of a systematic study of ZnO nanowire array growth to theoretical predictions, they found that ZnO nanowire growth closely follows the predictions of geometrical selection theory. This work will ultimately allow better control of creating ZnO structures with specific materials properties. This work was funded by the LLNL LDRD program. The image shows top views of the nanowires.

WITH CAMS, PLUTONIUM SORPTION MEASURED AT LOW CONCENTRATION

In a **paper published** in *Environmental Science & Technology*, LLNL researchers James Begg, Mavrik Zavarin, Pihong Zhao, Scott Tumey, and Annie Kersting, with Clemson University colleague (and former LLNL postdoc) Brian Powell, report measurements of the sorption of dissolved Pu^{5+} onto surfaces of a common clay mineral (sodium montmorillonite) over an unprecedentedly large range of initial Pu solution concentrations (10^{-6} to 10^{-16} M). Concentration measurements at the low end of this range were made possible by the unique capabilities of the LLNL Center for Accelerator Mass Spectrometry. The team's results show that the Pu adsorption behavior on montmorillonite was linear over the range of concentrations studied. This work answers a longstanding question about the validity of laboratory measurements of Pu sorption by indicating that Pu sorption behavior in at the higher concentrations of laboratory measurements can be extrapolated to sorption behavior at low, environmentally relevant concentrations.

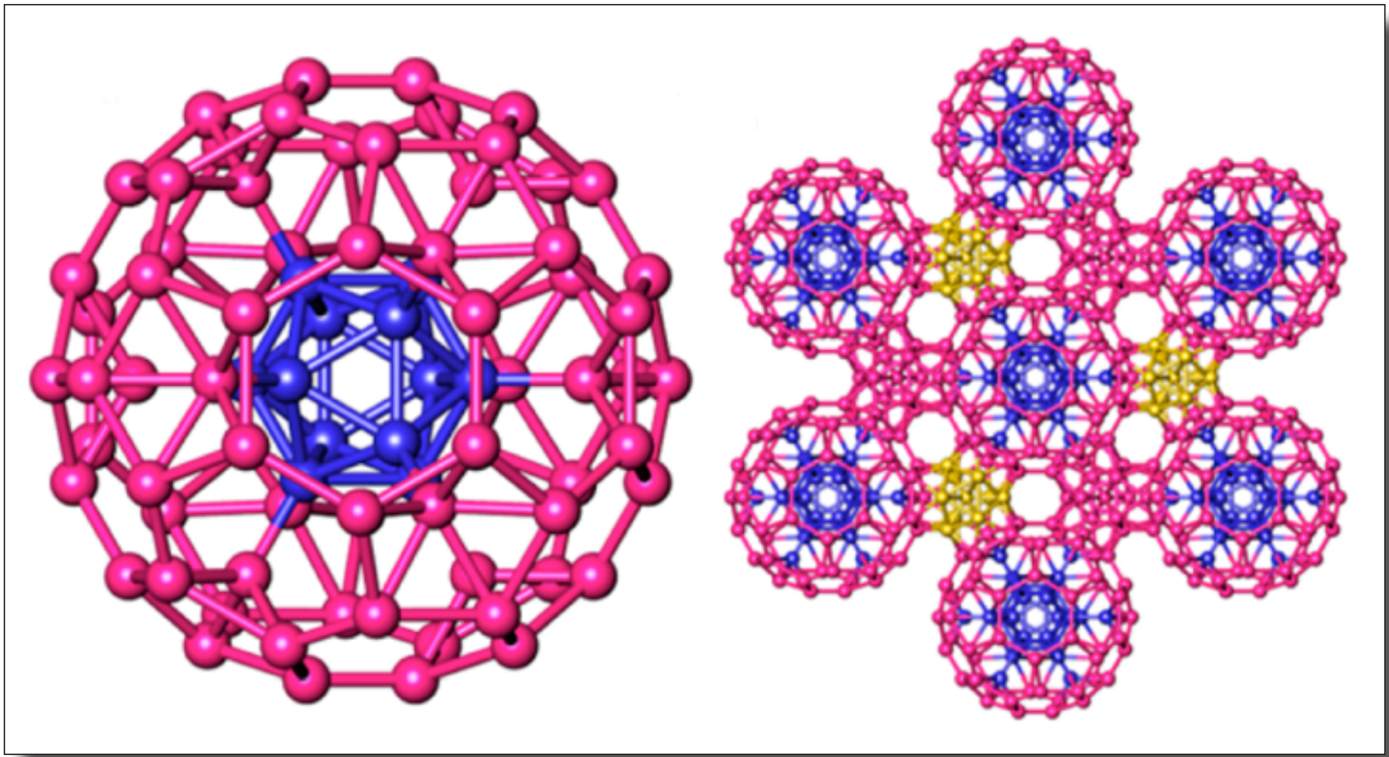


BORON AND THE "PHYSICS OF FRUSTRATION" REPORTED IN *CHEMICAL REVIEWS*

In an **invited article** in *Chemical Reviews*, LLNL researchers Tadashi Ogitsu and Eric Schwegler, along with Giulia Galli from UC Davis, discuss in detail the properties of beta boron, as inferred from experiments and the ab initio theories developed over the last decade. In the periodic table, boron occupies a peculiar, transitional position. It sits on the first row, and has metallic elements to its left and nonmetals to its right. Furthermore, it is the only nonmetal in the third column of the periodic table. It is therefore not surprising that the crystallographic structure and topology of boron's stable form at room temperature (β-boron) are not shared by any other element and are extremely complex. The formidable intricacy of β-boron, characterized by interconnecting icosahedra, partially occupied sites, and an unusually large number of atoms per unit cell (more than 300), has been known for more than 40 years. Surprisingly, boron remains the only element purified in macroscopic quantities for which the ground state geometry has not been completely determined by experiments. Theoretical progress over the last decade has shed light on numerous properties of elemental boron, leading to a thorough characterization of its structure at ambient conditions, as well as of its electronic and thermodynamic properties. The figure shows the 84-atom unit (B_{84}, left) that comprises beta-rhombohedral boron when multiple units are connected (right) by 10-atom units known as B_{10} (colored gold in the figure).

PCMDI WORK HIGHLIGHTED

A recent "Down to Earth" column of *Physics Today* **highlighted** a paper published in the Nov. 2, 2012 edition of *Geophysical Research Letters* and co-authored by Program for Climate Model Diagnosis and Intercomparison researchers Peter Gleckler, Benjamin Santer, and Paul Durack, with colleagues at the Scripps Institution of Oceanography. The paper—**previously highlighted** in the "Research Spotlight" section of *EOS*—shows that changes in ocean salinity over the second half of the 20th century are consistent with changes driven by human activities and are inconsistent with natural climate variations.



"IMPOSSIBLE" RADIOACTIVE DECAY MEASUREMENTS ENABLED BY NEW ION-TRAP SYSTEM

The online edition of *Physical Review Letters* recently published two papers describing experiments performed with an ion trap developed for precision beta-decay spectroscopy—a new apparatus that confines single radioactive ions in free space. Developed by LLNL physicist Nick Scielzo and collaborators across the U.S. and Canada, the device allows researchers to infer the properties of particles emitted in radioactive decays that are either difficult to detect (e.g., the neutron) or nearly impossible to detect (e.g., the neutrino) by measuring all the other (easier to detect) particles involved in the decay. This approach has the potential to revolutionize radioactive decay measurements.

The **first paper** describes a fundamentally new technique that circumvents the many limitations associated with studying neutron emission following nuclear beta decay by dispensing with neutron detection and instead studying the tiny recoil kick imparted to the nucleus from the decay. The authors show for the first time that it is possible to reconstruct the number and energies of the neutrons emitted by a decaying nucleus by measuring the time of flight of the recoiling daughter nuclei to a nearby detector.

The **second paper** reports the results of using the ion trap to study the particles emitted from the nuclear beta decay of ^{8}Li. Although the neutrino is virtually undetectable, by detecting all the other particles from the decay of ^{8}Li, the direction and energy of each emitted antineutrino was determined. The results of this experiment confirm current theory and pave the way for further measurements that will test the Standard Model with unprecedented precision.

These efforts were supported by Livermore's LDRD program and DOE's Office of Nuclear Physics.

AMS-COMPUTATIONAL STUDY OF YEAST UNCOVERS POSSIBLE MECHANISM OF TISSUE DAMAGE FROM EXCESS SUGAR CONSUMPTION

In a **recent paper** in the journal *Yeast*, Ben Stewart and colleagues at LLNL and Mercer University report that healthy cells of the yeast *Saccharomyces cerevisiae* can rapidly detoxify methylglyoxal. This toxic metabolite produced by the spontaneous degradation of the sugar metabolites known as triose phosphates can chemically modify macromolecules in cells, potentially disrupting cellular function, and so may play a role in the adverse effects of excessive sugar consumption on the human body. In this study, accelerator mass spectrometry measurements of carbon-14-labeled methylglyoxal were conducted at Livermore's Center for Accelerator Mass Spectrometry. Computational modeling showed that increased glucose consumption may cause a significant increase in methylglyoxal formation by depletion of the oxidized cofactor nicotinamide adenine dinucleotide, which is essential for the normal metabolism of triose phosphates. These findings suggest biochemical mechanisms by which tissue damage results from excess sugar intake and so may be applicable to not only human type-2 diabetes but also cancer and other diseases. Work at LLNL was funded in part by the LDRD program.

RESEARCHERS CONTRIBUTE CHAPTERS TO NEW VOLUME ON EARTH SYSTEM MODELING

Computation researchers Robert Drach and Dean Williams authored chapters in the fourth volume of the **book** *Earth System Modeling*. Robert was the chapter lead for **data representation**, and Dean was the chapter lead for **data analysis and visualization**.

NUCLEAR CHRONOMETER: TOOL FOR IDENTIFYING SOURCE OF INTERDICTED URANIUM?

Laboratory researchers Gary Eppich, Ross Williams, Amy Gaffney, and Kerri Schorzman are authors of a **paper published** in the *Journal of Analytical Atomic Spectrometry* that describes the utility of forensically dating uranium materials using the uranium 235–protactinium 231 chronometer to determine the "age" of the material—that is, the time since its most recent chemical purification. This information and other data yielded from nuclear forensic analysis can, together with conventional forensics, provide valuable insight into the source, destination, and suspected use of interdicted nuclear materials.

EMITTANCE OF POSITRON BEAMS MEASURED

The emittance values of positron beams produced by intense lasers have been measured for the first time by LLNL researchers and their collaborators. In a *Physics of Plasmas* **paper** lead-authored by LLNL's Hui Chen and chosen as a "Research Highlight," the researchers reported that the laser-produced positrons have a geometric emittance comparable to the positron sources used at existing accelerators. This low-emittance beam, which is quasi-monoenergetic in the energy range of 5 to 20 MeV, may be useful as an alternative positron source for future accelerators. The emittance values were derived through measurements of positron beam divergence and source size for different peak positron energies under various laser conditions. The experiments were performed using 10-picosecond laser pulses at 1.054-μm wavelength from LLNL's Titan laser and the OMEGA EP laser at the University of Rochester. Laser-produced positrons as a new source for accelerators offer the potential advantages of a much reduced physical size, lower cost, and improved beam characteristics: particles per pulse, energy span, and beam emittance. Work done at LLNL was supported by the LDRD Program.

MODE CONVERTER SYSTEM REPORTED IN *LASER FOCUS WORLD*

Fiber lasers have the potential to generate high average power with excellent beam quality and efficiency, compactness, and reliability. Fiber-laser amplifiers using conventional large-mode-area or photonic-crystal fibers can output a maximum of about 36 (kW) with ideal, diffraction-limited beam quality. LLNL researchers are working to increase the output of these lasers by changing the shape of the waveguide from a circularly symmetric fiber to a rectangular ("ribbon") fiber. The February 13 issue of *Laser Focus World* **describes** a mode-converter system that will enable rectangular-core fibers to extend single-aperture fiber-laser amplifier output to more than 100 kW while retaining diffraction-limited beam quality. The mode converter, developed by LLNL physicist Arun Sridharan and colleagues uses two diffractive optical elements—or "phase only" plates—implemented with spatial light modulators. "In the future," says Arun, "phase plates fabricated in fused-silica glass can be used to build the mode converter to withstand the high-power output from rectangular-core fiber amplifiers. These mode converters can also be leveraged for improved power extraction in bulk solid-state amplifiers."

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Questions? Comments?

Please contact Paul Kotta at **kotta1@llnl.gov** or (925) 424-4018.